2-Methylbutyl 8-methylnon-6-enoate

Inchi: InChI=1S/C15H28O2/c1-5-14(4)12-17-15(16)11-9-7-6-8-10-13(2)3/h8,10,13-14H,5-7,9,1
InchiKey: PLTRJLWIJLCEOL-CSKARUKUSA-N
Formula: C15H28O2
SMILES: CCC(C)COC(=O)CCCCC=CC(C)C
Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	-83.16	kJ/mol	Joback Method
hf	-491.07	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.348		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	1545.20		NIST Webbook
rinpol	1545.20		NIST Webbook
tb	622.17	K	Joback Method
tc	800.65	K	Joback Method
tf	295.89	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.34	J/mol×K	622.17	Joback Method
cpg	681.63	J/mol×K	770.90	Joback Method
cpg	667.11	J/mol×K	741.15	Joback Method
cpg	651.84	J/mol×K	711.41	Joback Method
cpg	635.80	J/mol×K	681.66	Joback Method
cpg	618.98	J/mol×K	651.92	Joback Method
cpg	695.44	J/mol×K	800.65	Joback Method
dvisc	0.0001019	Pa×s	622.17	Joback Method

dvisc	0.0001417	Pa×s	567.79	Joback Method
dvisc	0.0002114	Pa×s	513.41	Joback Method
dvisc	0.0003466	Pa×s	459.03	Joback Method
dvisc	0.0006492	Pa×s	404.65	Joback Method
dvisc	0.0014772	Pa×s	350.27	Joback Method
dvisc	0.0045474	Pa×s	295.89	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume